# Molecular Data for a Biochemical Model of DNA Damage: Electron Impact Ionization and Dissociative Ionization Cross Sections of DNA Bases and Sugar-Phosphate Backbone

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## Abstract

As part of the database for building up a biochemical model of DNA radiation damage, electron impact ionization cross sections of sugar-phosphate backbone and DNA bases have been calculated using the iBED model. It is found that the total ionization cross sections of $C_3$'- and $C_5$'-deoxyribose-phospate, two conformers of the sugar-phosphate backbone, are close to each other. Furthermore, the sum of the ionization cross sections of the separate deoxyribose and phosphate fragments is in close agreement with the $C_3$'- and $C_5$'-deoxyribose-phospate cross sections, differing by less than 10%. Of the four DNA bases, the ionization cross section of guanine is the largest, then in decreasing order, adenine, thymine, and cytosine. The order is in accordance with the known propensity of oxidation of the bases by ionizing radiation. Dissociative ionization (DI), a process that both ionizes and dissociates a molecule, is investigated for cytosine. The DI cross section for the formation of H and $(\text{cytosine-H1})^+$, with the cytosine ion losing H at the 1 position, is also reported. The threshold of this process is calculated to be 17.1 eV. Detailed analysis of ionization products such as in DI is important to trace the sequential steps in the biochemical process of DNA damage.

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## 1. Introduction

In radiation research, a biophysical model is frequently used to link the dosimetry of radiation with measurements of biological damages. Based on a stochastic approach and employing empirical data of energy deposition and molecular damage, Monte Carlo simulation has evolved to the stage that it becomes an important tool in the modeling and calculation of initial effects of radiation damage (*1,2*). Simultaneously, advances in experimental techniques have begun to provide information on the chemical processing that links the early physical events to the biological damage evolved later. It is therefore desirable to extend the modeling so as to provide the framework for analyzing such experimental data. So far, virtually all analyses of chemical processes are based on energetic considerations. Energetic studies can only provide information on the possibility, but not the probability, for a reaction to occur. More rigorous theoretical analysis, involving quantitative estimates of damage probability, is desirable. Such a model will have predictive capability and can be employed not just to understand the damage mechanism, but also the repair mechanism, and to propose possible countermeasures.

Due to the lack of atomistic detail, Monte Carlo track simulations cannot be easily adapted to include chemical processes. In a biochemical model, it is not only necessary to know the initial energy deposition and probability of damage, but also the chemical identity of the damage products so that it can predict the subsequent steps of the damage process. Chemical structures are an integral part in the simulation. Detailed microscopic data, including electron (δ-ray) collision cross-sections, chemical reaction rates, and transport properties, are needed for the modeling. So far only limited data are available.

The role of ionization in DNA damage is well recognized. The ionization (oxidation) of the deoxyribose sugar results not only in strand breaks, but also in the formation of a variety of electrophilic degradation products that can further react with proteins and DNA bases (*3*). The guanine radical cation is considered one of the precursors to the primary, direct-type lesions formed in DNA when it is irradiated *in vivo* (*4*). Up to the present, no experimental measurement of the cross sections of these moieties, and only one theoretical calculation (*5*), have been reported. Furthermore, dissociative ionization (DI), a process that simultaneously ionizes and dissociates a molecule, has never been used in analyzing direct DNA damage even though the OH radicals generated by the DI of water plays an important role in indirect damage mechanisms. As part of the molecular database to build up a biochemical model, this

paper reports total ionization cross sections, M + e → 2e + all products, for deoxyribose, phosphate, $C_3$'- and $C_5$'-deoxyribose-phosphate, and the four DNA bases. The total ionization cross section describes the probability of depositing electron energy on the target molecular species, producing a new electron. It does not provide the information regarding the nature of the molecular damage. To obtain details of the damage, studies such as DI are required. The first study of DI of a DNA base is also presented here.

## 2. Calculations and Results

The geometries of deoxyribose, phosphate, $C_3$'- and $C_5$'-deoxyribose-phosphate, and the four DNA bases guanine, adenine, thymine, and cytosine were determined with the Hartree-Fock (HF) method and the cc-pVTZ basis of Gaussian functions employing the *GAMESS* code (*6*). To simulate the electronegativity of phosphate in DNA, we use the anion structure $H_2PO_4^-$ instead of the neutral species. The two molecular properties used in the ionization cross section calculations (see discussion below) are the kinetic energies and ionization potentials of molecular electrons. The kinetic energies of the molecular electrons were calculated using HF functions because one-electron properties calculated using HF calculations are variationally stable to first order. For phosphate, deoxyribose, and thymine, the vertical ionization potential (VIP) of the outermost valence electron is calculated as the difference between the energies of the ion and the neutral molecule using the CCSD(T) method (couple-cluster singles and doubles with perturbation treatment of triples) (*7,8*) and the *MOLPRO* code (*9*). The CCSD(T) method is a size-consistent correlated treatment and has been shown to provide the most reliable data for the calculations of VIP. For all other VIPs, the HF values based on Koopmans theorem were used.

In the iBED (improved binary-encounter dipole) formulation (*10*), the electron impact ionization cross section is given by the sum of two terms: (i) a modified Mott cross section of Coulomb scattering with exchange, with the incident electron energy replaced by the average energy from the binary encounter model, and (ii) the dipole Born cross section that describes the dipole interaction between the scattering electron and the target. While the modified Mott cross section describes the close collisions important at low electron energies, the dipole Born cross section describes the long range dipole interaction that dominates at high energies. Note, however, the dipole interaction potential used in the iBED formulation has a shielding term that describes the repulsive interaction as the scattering electron enters into the bonding region. This shielding term

has been found to play an important role in obtaining reliable cross sections in electron collisions with radicals (*11,12*).

The iBED formulation differs from the BEB (Binary-Encounter Bethe) model developed by Kim and Rudd (*13*) in several aspects. The BEB treatment uses the Bethe dipole cross section to represent the high-energy limit of the dipole interaction where only the long range dipole potential is important. The iBED treatment, on the other hand, not only describes the long-range electron-target dipole interaction, but also the shielding of the dipole field as the scattering electron comes inside the bonding region. In addition, in the iBED formulation the optical oscillator strength used in the dipole interaction depends on the ejected electron energy as $E_p^{-3.5}$, an energy dependence derived by theoretical analysis. The BEB formulation, on the other hand, uses $E_p^{-3}$ energy dependence. As an illustration of the quality of the data generated by the iBED method, Fig. 1 presents the total ionization cross section of water, $H_2O + e \rightarrow 2e +$ all products, calculated using the iBED method, the BEB method and the experimental data of Straub *et al.* (*14*) and Schutten *et al.* (*15*). The measurements of Straub *et al.* are considered the most accurate, with an estimated error of ±5%, whereas the older data by Schutten *et al.*, with an estimated error of ±15%, extend to higher energies. Two sets of iBED cross sections are presented, one with the optical oscillator strength $f_o$ from the photoionization data of Brion *et al.* (*16*), and the second with $f_o$ determined using the Thomas-Reich-Kuhn sum rule. The two iBED cross sections are in agreement with each other and with both sets of experimental data. The BEB cross sections are calculated using the same set of molecular electron kinetic energies and ionization potentials as the iBED calculations and they are found to be ≈20% larger than both the iBED cross sections and experimental measurements.

**(a). Total electron impact ionization cross sections of deoxyribose, phosphate, and $C_3$'- and $C_5$'-deoxyribose-phosphate**

Figure 2 presents the structure of the phosphate ($H_2PO_4^-$, denoted as $Ph^-$), deoxyribose sugar ($C_5H_{10}O$) and two conformations of the sugar-phosphate backbone, $C_3$'- and $C_5$'-deoxyribose-phosphate ($C_5H_{10}O_5P^-$, denoted as $C_3$-$Ph^-$ and $C_5$-$Ph^-$, respectively), depending on the location of the sugar–phosphate bond. In our preliminary calculations, the electronegativity of the phosphate group in the sugar-phosphate backbone is simulated by the use of the phosphate anion. In a previous study of the DNA backbone, Bernhardt and Paretzke (*5*) performed calculations of the DNA backbone in the presence of a $Na^+$ counter ion. Unlike the calculation of Bernhardt

and Paretzke (*5*), a counter ion is not used in our wave function calculations of $Ph^-$, $C_3'$-$Ph^-$ and $C_5'$-$Ph^-$. Thus the calculated first VIPs for these three species are lower than those obtained by Bernhardt and Paretzke. For $Ph^-$ the calculated first VIP using CCSD(T)/cc-pVTZ (CCSD(T) method and cc-pVTZ Gaussian basis) is 4.7 eV. For $C_3'$-$Ph^-$ and $C_5'$-$Ph^-$ they are 4.8 and 4.7 eV, respectively, using the HF/cc-pVTZ basis. By comparison, the first VIP of the sugar-phosphate backbone determined by Bernhardt and Paretzke using a sodium counter ion is 10.58 eV at the HF/3-21G level. The first VIP of deoxyribose, a neutral species, from the present CCSD(T)/cc-pVTZ calculation is 9.7 eV, also significantly higher than the anion VIPs. Thus the present calculation gives too low a VIP for $Ph^-$, $C_3'$-$Ph^-$, and $C_5'$-$Ph^-$ due to the use of anions without the presence of a counter ion. In future calculations counter ions will be included in order to compare our data directly with Bernhardt and Paretzke. Nevertheless, the major conclusions drawn from these calculations, as discussed below, are expected to remain valid.

Figure 3 presents the ionization cross sections of $Ph^-$, deoxyribose, $C_3'$-$Ph^-$ and $C_5'$-$Ph^-$ using the iBED method. The close spacing of the cross sections for $C_3'$-$Ph^-$ and $C_5'$-$Ph^-$ suggests that the total ionization cross section is insensitive to the location of the $Ph^-$-deoxyribose bond. However, the individual ionization channels corresponding to specific bond-breaking processes such as DI are expected to be more sensitive to the $Ph^-$-deoxyribose bonding site. Future studies will address this issue. In addition, the sum of the $Ph^-$ and deoxribose cross sections are close to the $C_3'$-$Ph^-$ and $C_5'$-$Ph^-$ cross sections. This appears to indicate that a building-up principle, where the total ionization cross section can be obtained from summing the ionization cross section of individual DNA functional groups. Further tests of the building-up principle will be carried out in the future.

Using the BEB (*13*) and DM (*17*) formulations, Bernhardt and Paretzke (*5*) reported total electron impact ionization cross sections of the sugar-phosphate backbone. The $C_3'$-$Ph^-$ and $C_5'$-$Ph^-$ total ionization cross sections using the iBED method are larger than the cross sections reported by Bernhardt and Paretzke by ~ 25%. Based on the water calculation in Fig. 1, it is expected that the iBED cross section should be smaller than the BEB result, instead of larger. The major source of this difference comes from the use of the anion without the presence of a counter ion. Future calculations including a counter ion will resolve this discrepancy.

**(b). Total electron impact ionization cross sections of DNA bases**

The first VIP of guanine calculated using HF/cc-pVTZ is 8.24 eV. This is to be compared with the experimental values of 8.24±0.03 (*18*), 8.0±0.2 (*19*), and 7.85 eV

(*20*). For adenine the calculated first VIP using HF/cc-pVTZ is 8.50 eV, versus the experimental values of 8.44±0.03 (*18*), 8.48 (*21,22*), 8.3±0.1 (*19*), and 8.9±0.1 eV (*23*). The calculated first VIP for thymine using CCSD(T)/cc-pVTZ is 8.78 eV, versus the experimental values of 9.14±0.03 (*18*), 9.0±0.1 (*19*), 9.4±0.1 (*23*), 9.20 (*20*), and 9.02 eV (*24*). The calculated value of the first VIP of cytosine using HF/cc-pVTZ is 9.31 eV, versus experimental values of 8.94±0.03 (*18*), 9.0±0.1 (*19*), 8.9±0.2 (*23*), and 8.45 eV (*20*).

Figure 4 presents the total ionization cross sections of guanine, adenine, thymine, and cytosine calculated using the iBED formulation. Of the four DNA bases, the ionization cross section of guanine is the largest, then in decreasing order, adenine, thymine, and cytosine. The order is in accordance with the known propensity of oxidation of the four bases by ionizing radiation. The iBED cross sections are ≈ 20% smaller than the BEB cross sections of Bernhardt and Paretzke (*5*), consistent with the deviations found in water.

**(c). Dissociative ionization cross sections of cytosine**

The ionization cross sections presented in Sec. (2a) and (2b) are total cross sections for the process M + e → 2e + all products. The only uniquely identified product in the process is a new, ejected electron. All other products are unidentified. For example, in the case of water, the products including in the total ionization cross sections are $H_2O^+$, $OH^+$, $H^+$, $H_2^+$, $O^+$, OH, H, $H_2$, and O. Thus the total ionization cross section corresponds to the probability of an energy deposition process by δ-rays, but does not provide the information regarding the nature of the damage. As a result, it cannot be deduced from the total ionization cross section what is the next step in the damage process. For example, it is known that the guanine cation is reactive, but the cytosine cation is less so. However, a cytosine radical cation, with one hydrogen removed, may well be much more reactive than cytosine cation itself. The biochemical model that we plan to develop requires data for the individual ionization process, including detailed information of ionization products. As a step in developing the necessary data, calculations of the DI of cytosine have been carried out,

$$\text{Cytosine} + e \rightarrow 2e + (\text{Cytosine} - H1)^+ + H. \qquad (1)$$

The cation $(\text{Cytosine} - H1)^+$ produced, corresponds to the parent cation $\text{Cytosine}^+$ with a hydrogen atom from the H1 position removed. Figure 5 illustrates the H1 position in cytosine and presents the DI cross section. The threshold of this process is 17.1 eV, significantly higher than the first VIP of cytosine. This is the first study of DI

process in DNA damage. The biochemical reactions that may occur due to the subsequent reaction of (Cytosine – H1)$^+$ will be the subject of future studies.

### 3. Discussions

The first set of molecular data for the development of a biochemical model of DNA radiation damage is presented here. The iBED method used for the calculation of electron impact ionization cross sections is first validated with a calculation of the water ionization cross section. The method is then applied to calculate the total ionization cross sections of DNA functional groups including Ph$^-$, dexoyribose sugar, and two conformers of the sugar-phosphate backbone, $C_3$'-Ph$^-$ and $C_5$'-Ph$^-$, and the four DNA bases. The calculations of the sugar, phosphate, and sugar-phosphate backbone series found that the ionization cross sections of the two sugar-phosphate backbones are very close to each other. Furthermore, the sum of the sugar and phosphate cross sections are within 10% of the sugar-phosphate backbone cross section. This evidence suggests that for certain processes in DNA, the interaction is localized and we can study the system by treating smaller fragments at higher levels of accuracy. This "building-up principle" if validated in future calculations, should expedite the development of the biochemical model.

Calculations of the total ionization cross sections of the four DNA bases show that guanine has the largest cross section, then in descending order, adenine, thymine, and cytosine. This order agrees with the experimental observed oxidation propensity of the bases by ionizing radiation. The present set of cross sections for the DNA bases is ~ 20% smaller than the BEB and DM cross sections of Bernhardt and Paretzke (*5*), consistent with the deviations found in water.

The present study presents the first DI cross section of a DNA base. This type of detailed study of the ionization processes that tracks the nature of the molecular products will enable us to trace the sequential biochemical steps in the mechanism of radiation damage and develop a more rigorous biochemical model.

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## Figure captions

Figure 1. Total single ionization cross-section of water, $H_2O + e \rightarrow 2e +$ all products. The green curve shows iBED cross sections determined using the optical oscillator strength from the photoionization data of Brion *et al.* (*16*). The blue curve presents iBED results where the Thomas-Reich-Kuhn sum rule is used to determine the optical oscillator strength. BEB cross sections are given by the red curve. The experimental data of Straub *et al.* (*14*) are represented by black circles and the data of Shutten *et al.* (*15*) are given by green triangles.

Figure 2. Molecular structures of the phosphate anion ($H_2PO_4^-$), deoxyribose sugar ($C_5H_{10}O$), and two conformers of the sugar-phosphate backbone, $C_3$'- and $C_5$'-deoxyribose-phosphate.

Figure 3. Total electron impact ionization cross sections of the phosphate anion, deoxyribose, and two conformers of the sugar-phosphate backbone, $C_3$'- and $C_5$'-deoxyribose-phosphate, calculated using the iBED formulation. Also presented in the orange dotted curve is the sum of phosphate and deoxyribose ionization cross sections.

Figure 4. Total electron impact ionization cross sections of the DNA bases guanine, adenine, thymine, and cytosine calculated using the iBED formulation.

Figure 5. Dissociative ionization cross section of the process Cytosine + e → 2e+ $(\text{Cytosine} - \text{H1})^+ + \text{H}$. The position of H1 in cytosine is also illustrated.

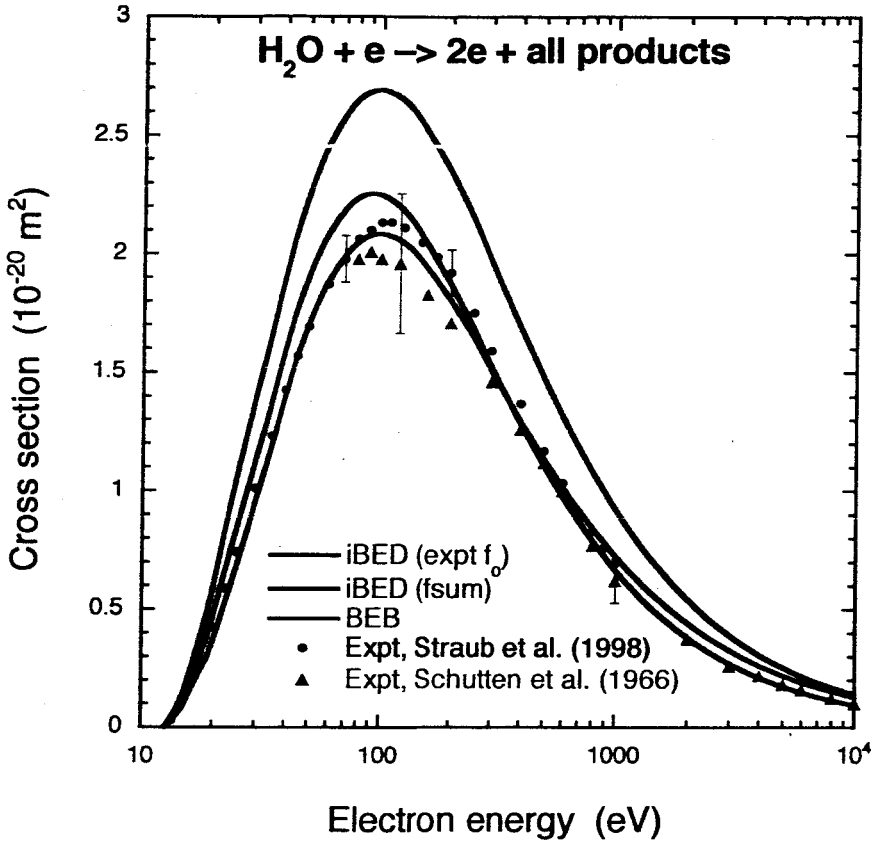
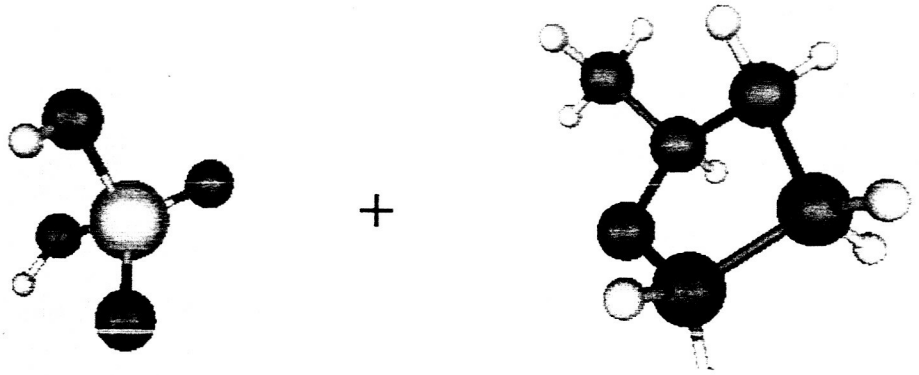

H2O + e -> 2e + all products
Cross section (10-20 m2)
Electron energy (eV)
iBED (expt f0)
iBED (fsum)
BEB
Expt, Straub et al. (1998)
Expt, Schutten et al. (1966)
0
0.5
1
1.5
2
2.5
3
10
100
1000
10^4

Figure 1

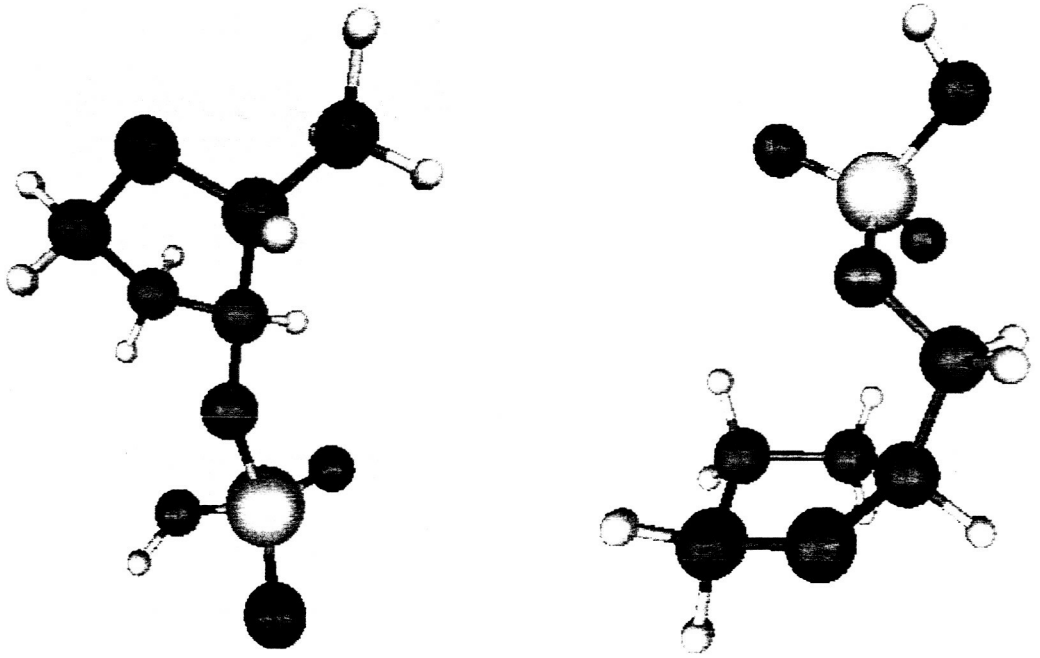


Phosphate
($H_2PO_4^-$)
$Ph^-$

+

Deoxyribose
($C_5H_{10}O$)

↓



$C_3'—Ph^-$
($C_5H_{10}O_5P^-$)

$C_5'—Ph^-$
($C_5H_{10}O_5P^-$)

Figure 2

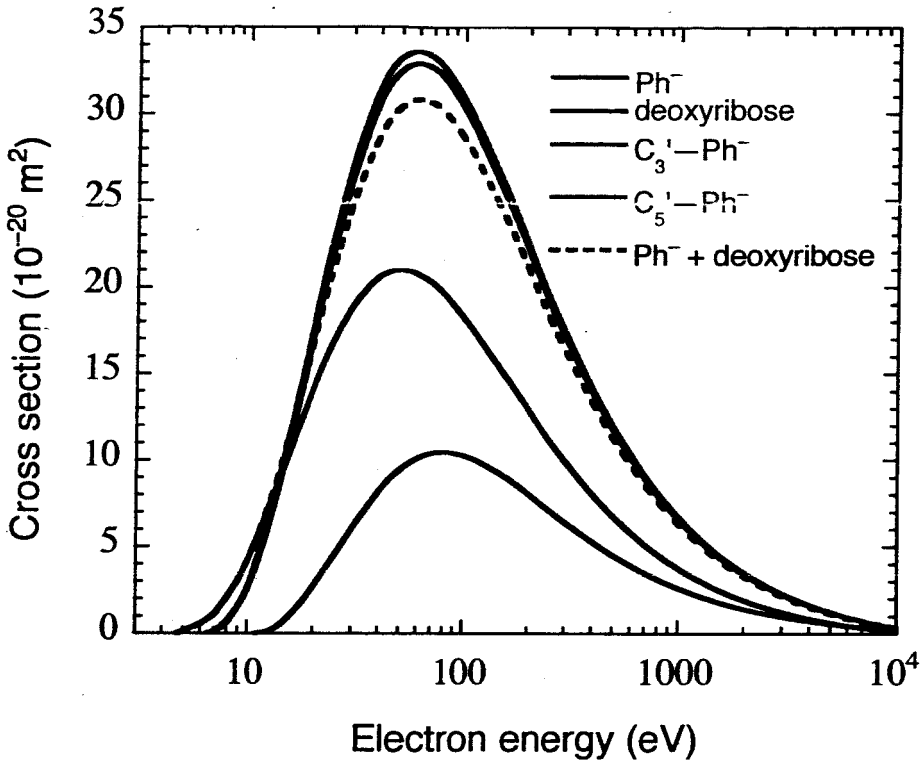

35
30
25
20
15
10
5
0
Cross section ($10^{-20}$ m$^2$)
10
100
1000
$10^4$
Electron energy (eV)
Ph⁻
deoxyribose
C3'—Ph⁻
C5'—Ph⁻
Ph⁻ + deoxyribose

Figure 3

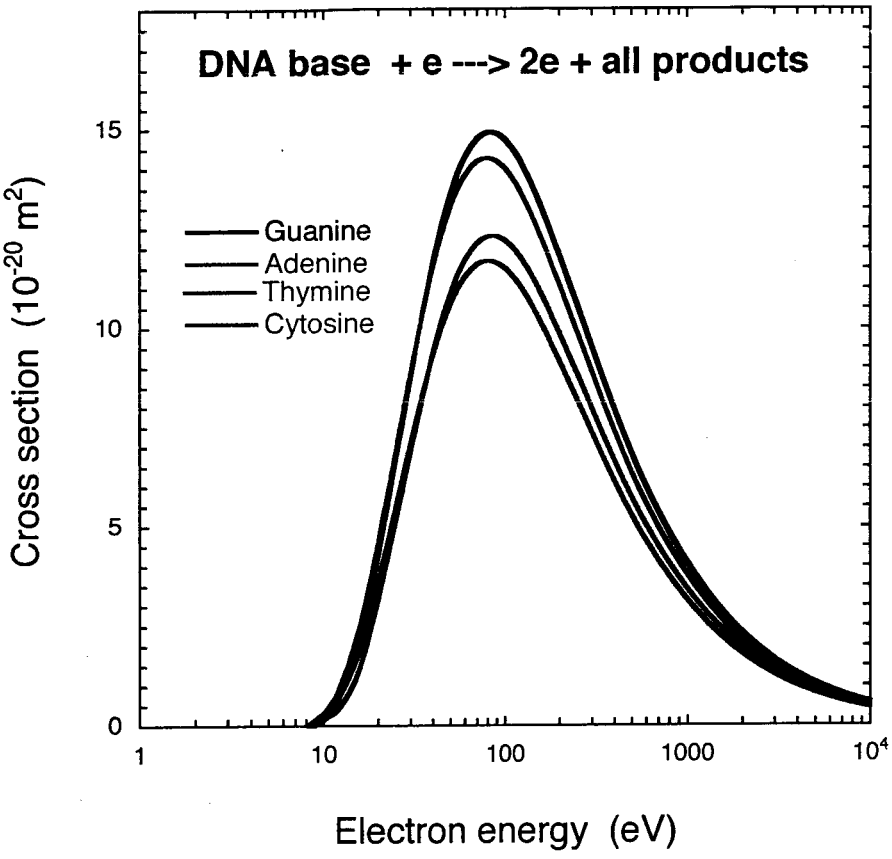
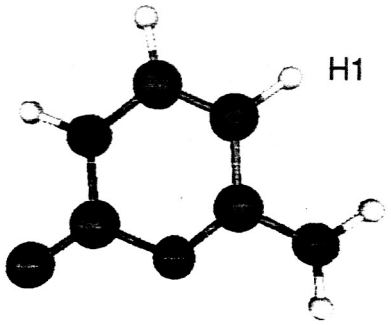

DNA base + e ---> 2e + all products
Guanine
Adenine
Thymine
Cytosine
Cross section ($10^{-20}$ m$^2$)
0
5
10
15
1
10
100
1000
$10^4$
Electron energy (eV)

Figure 4


H1

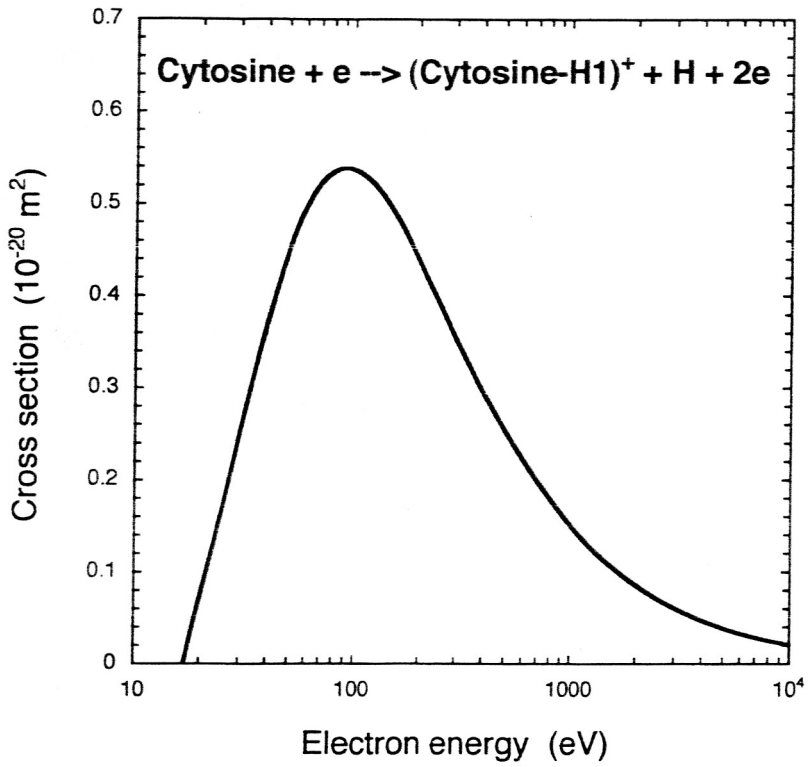

Cytosine + e --> (Cytosine-H1)+ + H + 2e
Cross section (10-20 m2)
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
10
100
1000
10^4
Electron energy (eV)

Figure 5